

## Benjamin F. Gherman

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### CURRENT EMPLOYMENT

- **California State University, Sacramento.** Sacramento, California, 2006-present.
  - **Assistant Professor**, September 2006-present.
    - Classes Taught: General Chemistry I, Physical Chemistry Lecture I and II, Introduction to Physical Chemistry, Computational Chemistry.
    - Research Focus: Computational bioinorganic, organometallic, and organic chemistry.

### EDUCATION

- **University of Minnesota (Twin Cities)**, Minneapolis, Minnesota, 2003-2006.
  - **Post-doctoral associate**, September 2003-July 2006.
    - Project Title: Modeling Oxygen Activation by Monocopper Enzyme Sites
- **Columbia University**, New York, New York, 1998-2003.
  - **Ph. D.** Chemistry, October 2003.
    - Dissertation Title: Using Quantum Chemical and Mixed Quantum Chemical/ Molecular Mechanics Methods to Study Reaction Mechanisms in Enzymes
    - Advisor: Richard A. Friesner
  - **M. Phil.** Chemistry, February 2002.
  - **M. A.** Chemistry, October 1999.
- **Carnegie Mellon University**, Pittsburgh, Pennsylvania, 1994-1998.
  - **B. S.** Chemistry (with Computational Chemistry option), May 1998.
  - **B. S.** Mathematics, May 1998.

### PROFESSIONAL EXPERIENCE

#### *Research Experience*

- **Post-doctoral Research**, *Department of Chemistry, University of Minnesota (Twin Cities).*
  - September 2003 – July 2006. Professor Christopher J. Cramer and Professor William B.

Tolman, advisors.

- ♦ Studied the catalytic mechanisms of the dopamine  $\beta$ -monooxygenase (D $\beta$ M) and peptidylglycine  $\alpha$ -hydroxylating monooxygenase (PHM) enzymes by quantum chemical modeling of the active sites. The effects of different coordination environments for the copper atoms on dioxygen activation and substrate hydroxylation are determined. This work represents the first application of theoretical methods to model specific reaction mechanisms in these enzymes and will greatly increase understanding of the reaction chemistry of monocopper complexes in general.
- ♦ Modeled dioxygen activation and substrate hydroxylation in biomimetic monocopper complexes being developed in the Tolman group. This work was carried out in conjunction with parallel experimental studies in the Tolman group.
- ♦ Mentored and collaborated with an undergraduate student as a part of these two projects, leading to publication (see #3 in publications).

• **Graduate Research**, *Department of Chemistry, Columbia University.*

· January 1999 – August 2003. Professor Richard A. Friesner, advisor.

- ♦ Based upon *ab initio* quantum chemical studies on a large-scale model, proposed for the first time complete and realistic catalytic cycles for dioxygen activation and methane hydroxylation by soluble methane monooxygenase, a metalloenzyme that is found in methanotrophic bacteria. Computational results were found to be fully consistent with and provide explanation for experimental data. Further work on this system succeeded in explaining the different rates and kinetic isotopic effects seen in the reaction of methane monooxygenase with substituted methane substrates.
- ♦ Use of a novel mixed quantum mechanics/molecular mechanics method (QM/MM) to determine the origin of the different rates for the deacylation step in the hydrolysis of  $\beta$ -lactam antibiotics performed by penicillin-binding proteins and class-C  $\beta$ -lactamases. This research played a role in understanding the differences in reactivity of the two enzymes towards  $\beta$ -lactam antibiotics and contributed to an understanding of the mechanism of bacterial antibiotic resistance.

• **Undergraduate Research**, Department of Chemistry, Carnegie Mellon University.

· May 1995 - August 1995, May 1996 - August 1996, May 1997 - August 1997, January 1998 - May 1998. Professor David Yaron, advisor.

- ♦ Studied the electronics of conjugated polymers (in particular, polyacetylene) using semi-empirical quantum methods and developed C++ computer code to implement the semi-empirical INDO quantum chemical method.

## ***Teaching Experience***

- **Course Assistant**, *Department of Chemistry, Columbia University*.
  - General Chemistry I and II, January 2000 - May 2001. Aided in various aspects of the courses, including:
    - ♦ maintaining the course web page
    - ♦ assisting in exam preparations and administrations
    - ♦ advising teaching assistants
    - ♦ answering questions on the class electronic bulletin board
- **Teaching Assistant**, *Department of Chemistry, Columbia University*.
  - August 1998 - December 1999. Taught general chemistry I and II recitations.
- **Teaching Assistant**, *Department of Mathematics, Carnegie Mellon University*.
  - August 1996 - May 1997. Taught calculus I and II recitations.

## ***Teaching Development***

- **Center for Teaching and Learning Services, University of Minnesota (Twin Cities)**.
  - *Preparing Future Faculty Program*, letter of recognition and certificate of program participation, December 2005.
  - “*Practicum for Future Faculty*” graduate course in the *Preparing Future Faculty Program*, September 2005 – December 2005.
    - ♦ Designed to give opportunities to apply pedagogical theories and methods and to enhance understandings of the faculty role in higher education. Includes a mentoring opportunity in which participants teach three class sessions and explore the faculty role with the guidance of a faculty mentor (at Augsburg College, Minneapolis, MN under Prof. Arlin Gyberg, Chemistry Dept.).
  - “*Using Electronic Discussions*” workshop, April 2005.
    - ♦ Included topics such as asynchronous (threaded) online discussions and the ways they may be used in face-to-face classes.
  - “*PowerPoint Reconsidered*” workshop, March 2005.
    - ♦ Included topics such as common problems when teaching with PowerPoint and pedagogically sound ways use to this presentation technology.
  - “*Teaching in Higher Education*” graduate course in the *Preparing Future Faculty Program*, September 2004 – December 2004.
    - ♦ Included topics such as active learning strategies, educational theory and practice, diversity of learners, and course and curriculum design. Designed with overall goal

of training responsive and reflective teachers.

· *Preparing Future Faculty Retreat*, May 2004

- ◆ Included workshops on “E-tivities: Engaging Students with Technology” and “Presenting Content: Lively & Practical Approaches”

• **Graduate School of Arts and Sciences, Columbia University.**

· *Teaching Program Workshop*, October 2001. “Teaching: Course Web Pages and Courseworks”

**AWARDS**

- California State University, Sacramento College of Natural Sciences and Mathematics faculty promotion development grant, 2011.
- California State University, Sacramento research and creativity award, 2011.
- California State University, Sacramento pedagogy enhancement award, 2011.
- California State University CSUPERB faculty-student collaborative research seed grant, 2010.
- California State University, Sacramento pedagogy enhancement award, 2010.
- California State University, Sacramento College of Natural Sciences and Mathematics faculty promotion development grant, 2010 (twice).
- California State University, Sacramento College of Natural Sciences and Mathematics faculty travel grant, 2009.
- California State University, Sacramento research and creativity award, 2009.
- California State University, Sacramento pedagogy enhancement award, 2009.
- California State University, Sacramento probationary faculty development grant, 2008.
- California State University, Sacramento College of Natural Sciences and Mathematics, summer project grant, 2008.
- California State University, Sacramento research and creativity award, 2008.
- California State University, Sacramento pedagogy enhancement award, 2008.
- Wiley-International Journal of Quantum Chemistry Young Investigator Award, 2008.
- California State University, Sacramento University Enterprises, Inc., faculty professional development award, 2008.
- California State University CSUPERB faculty travel grant (twice), 2008.
- Developmental project allocation (title: “Using Mixed Quantum Mechanics/Molecular Mechanics Calculations to Assess the Effects of Mutations on the Catalytic Activity of Peptide Deformylase”) of 24,000 service units from the National Center for Supercomputing Applications (NCSA), 2007-2008.
- NIH National Research Service Award Post-doctoral Fellowship, titled “Modeling Oxygen Activation by Monocopper Enzyme Sites,” 2003-2006.

- NIH Biophysics Training Grant, Columbia University, 2001-2003.
- Jack Miller Award for graduate teaching, Columbia University, 2000.
- U.S. Department of Defense National Defense Science and Engineering Graduate Fellowship, Columbia University, 1998-2001.
- Member Phi Beta Kappa Honor Society, Carnegie Mellon University, 1998.
- College awardee of the Society of Analytical Chemists of Pittsburgh, Carnegie Mellon University, 1998.
- Lubrizol scholarship for chemistry majors, Carnegie Mellon University, 1997.
- Warner Prize for sophomore chemistry majors, Carnegie Mellon University, 1996.
- Member Phi Kappa Phi Honor Society, Carnegie Mellon University, 1996.
- Member Lambda-Sigma National Sophomore Honor Society, Carnegie Mellon University, 1995 and Hall of Fame member, 1996.
- University scholarship, Carnegie Mellon University, 1995-1998.
- Dean's high honor list, Carnegie Mellon University, all four academic years 1994-1998.

## **PUBLICATIONS**

(undergraduate students denoted with asterisk)

1. N. G. Spiropulos, E. A. Standley, I. R. Shaw, B. L. Ingalls, B. Diebels, S. V. Krawczyk\*, B. F. Gherman, A. M. Arif, E. C. Brown. "Synthesis of Zinc and Cadmium *O*-Alkyl Thiocarbonate and Dithiocarbonate Complexes and a Cationic Zinc Hydrosulfide Complex." Manuscript in preparation.
2. N. V. Korovina\*, M. L. Chang\*, T. T. Nguyen\*, H. J. Walker, R. P. Fernandez\*, M. M. Olmstead, B. F. Gherman, J. D. Spence. "Syntheses and Reactivity of Naphthalenyl-Substituted Arenediyne." *Org. Lett.*, **13**, 3660-3663 (2011).
3. M. F. Brown\*, B. F. Gherman. "Importance of Iron as the Metal Ion in Peptide Deformylase: A Biomimetic Computational Study." *Theor. Chem. Acc.*, **128**, 137-146 (2011).
4. S. B. Bateni\*, K. R. England\*, A. T. Galatti\*, H. Kaur\*, V. A. Mendiola\*, A. R. Mitchell\*, M. H. Vu\*, B. F. Gherman, J. A. Miranda. "Prediction of Reduction Potentials from Calculated Electron Affinities for Metal-Salen Compounds." *Beilstein J. Org. Chem.*, **5** (2009), doi:10.3762/bjoc.5.82.
5. B. F. Gherman and C. J. Cramer. "Quantum Chemical Studies of Molecules Incorporating a Cu<sub>2</sub>O<sub>2</sub><sup>2+</sup> Core." *Coord. Chem. Rev.*, **253**, 723-753 (2009).
6. A. H. Winter, D. E. Falvey, C. J. Cramer, B. F. Gherman. "Benzylic Cations with Triplet Ground States: Computational Studies of Aryl Carbenium Ions, Silylenium Ions, Nitrenium Ions and Oxenium Ions Substituted with *meta* Pi Donors." *J. Am. Chem. Soc.*, **129**, 10113-10119 (2007).
7. N. E. Schultz, B. F. Gherman, C. J. Cramer, D. G. Truhlar. "Pd<sub>n</sub>CO (*n* = 1,2): Accurate ab Initio Bond Energies, Geometries, and Dipole Moments and the Applicability of Density Functional Theory for Fuel Cell Modeling." *J. Phys. Chem. B*, **110**, 24030-24046 (2006).
8. L. R. M. Hill, B. F. Gherman, N. W. Aboelella, C. J. Cramer, W. B. Tolman. "Electronic Tuning of

- $\beta$ -Diketimate Ligands with Fluorinated Substituents: Effects on the O<sub>2</sub>-Reactivity of Mononuclear Cu(I) Complexes.” *Dalton Trans.* 4944-4953 (2006).
9. D. E. Heppner, B. F. Gherman, W. B. Tolman, C. J. Cramer. “Can an Ancillary Ligand Lead to a Thermodynamically Stable End-on 1:1 Cu-O<sub>2</sub> Adduct Supported by a  $\beta$ -Diketimate Ligand?” *Dalton Trans.* 4773-4782 (2006).
  10. B. F. Gherman, W. B. Tolman, C. J. Cramer. “Characterization of the Structure and Reactivity of Monocopper-Oxygen Complexes Supported by  $\beta$ -Diketimate and Anilido-Imine Ligands.” *J. Comput. Chem.* **27**, 1950-1961 (2006).
  11. N. W. Aboeella, B. F. Gherman, L. M. Hill, J. T. York, N. Holm, V. G. Young, Jr., C. J. Cramer, W. B. Tolman. “Effects of Thioether Substituents on the O<sub>2</sub> Reactivity of  $\beta$ -Diketimate-Cu(I) Complexes: Probing the Role of the Methionine Ligand in Copper Monooxygenases.” *J. Am. Chem. Soc.* **128**, 3345-3358 (2006).
  12. B. F. Gherman, D. E. Heppner, W. B. Tolman, C. J. Cramer. “Models for Dioxygen Activation by the Cu<sub>B</sub> Site of D $\beta$ M and PHM.” *J. Biol. Inorg. Chem.* **11**, 197-205 (2006).
  13. C. R. Kinsinger, B. F. Gherman, L. Gagliardi, C. J. Cramer. “How Useful Are Vibrational Frequencies of Isotopomeric O<sub>2</sub> Fragments for Assessing Local Symmetry? Some Simple Systems and the Vexing Case of a Galactose Oxidase Model.” *J. Biol. Inorg. Chem.* **10**, 778-789 (2005).
  14. A. M. Reynolds, B. F. Gherman, C. J. Cramer, W. B. Tolman. “Characterization of a 1:1 Cu/O<sub>2</sub> Adduct Supported by an Anilido-Imine Ligand.” *Inorg. Chem.* **44**, 6989-6997 (2005).
  15. N.W. Aboeella, W. W. Brennessel, V. G. Young, Jr., S. Kryatov, E. Rybak-Akimova, R. Sarangi, E. I. Solomon, B. F. Gherman, C. J. Cramer, and W. B. Tolman. “Dioxygen Activation at a Single Copper Site: Structure, Bonding, and Mechanism of Formation of 1:1 Cu/O<sub>2</sub> Adducts.” *J. Am. Chem. Soc.* **126**, 16896-16911 (2004).
  16. B. F. Gherman and C. J. Cramer. “Modeling the Peroxide/Superoxide Continuum in 1:1 Side-on Adducts of O<sub>2</sub> with Cu.” *Inorg. Chem.* **43**, 7281-7283 (2004).
  17. B. F. Gherman, S. J. Lippard, and R. A. Friesner. “Substrate hydroxylation in methane monooxygenase: quantitative modeling via mixed quantum mechanics/molecular mechanics techniques.” *J. Am. Chem. Soc.* **127**, 1025-1037 (2005).
  18. B. F. Gherman, S. Goldberg, V. W. Cornish, and R. A. Friesner. “Mixed Quantum Mechanical/Molecular Mechanical (QM/MM) Study of the Deacylation Reaction in a Penicillin Binding Protein (PBP) Versus in a Class C  $\beta$ -Lactamase.” *J. Am. Chem. Soc.* **126**, 7652-7664 (2004).
  19. B. F. Gherman, S. J. Lippard, and R. A. Friesner. “Dioxygen activation in methane monooxygenase: a theoretical study.” *J. Am. Chem. Soc.* **126**, 2978-2990 (2004).
  20. R. A. Friesner, M.-H. Baik, V. Guallar, B. F. Gherman, M. Wirstam, R. B. Murphy, and S. J. Lippard. “How iron-containing proteins control dioxygen chemistry: a detailed atomic level description via accurate quantum chemical and mixed quantum mechanics/molecular mechanics calculations.” *Coord. Chem. Rev.* **238-239**, 267-290 (2003).

21. M.-H. Baik, B. F. Gherman, R. A. Friesner, and S. J. Lippard. "Hydroxylation of methane by non-heme diiron enzymes. A molecular orbital analysis of C-H bond activation by reactive intermediate Q." *J. Am. Chem. Soc.* **124**, 14608-14615 (2002).
22. V. Guallar, B. F. Gherman, S. J. Lippard, and R. A. Friesner. "Quantum chemical studies of methane monooxygenase: comparison with P450." *Curr. Opin. Chem. Biol.* **6**, 236-242 (2002).
23. V. Guallar, B. F. Gherman, W. H. Miller, S. J. Lippard, and R. A. Friesner. "Dynamics of alkane hydroxylation at the non-heme diiron center in methane monooxygenase." *J. Am. Chem. Soc.* **124**, 3377-3384 (2002).
24. B. F. Gherman, B. D. Dunietz, D. A. Whittington, S.J. Lippard, and R. A. Friesner. "Activation of the C-H bond of methane by intermediate Q of methane monooxygenase: a theoretical study." *J. Am. Chem. Soc.* **123**, 3836-3837 (2001).
25. B. F. Gherman, R. A. Friesner, T.-H. Wong, Z. Min, and R. Bersohn. "Photodissociation of acetaldehyde: the CH<sub>4</sub> + CO channel." *J. Chem. Phys.* **114**, 6128-6133 (2001).
26. I. Ivanov, B. F. Gherman, and D. Yaron. "Comparison of the INDO band structures of polyacetylene, polythiophene, polyfuran, and polypyrrole." *Synthetic Metals* **116**, 111-114 (2001).
27. E. Moore, B. F. Gherman, and D. Yaron. "Coulomb screening and exciton binding energies in conjugated polymers." *J. Chem. Phys.* **106**, 4216-4227 (1997).
28. D. Yaron, E. Moore, and B. F. Gherman. "Models of electron-hole screening and exciton binding in conjugated polymers." *Materials Research Society Symposium Proceedings* **413**, 541-546 (1996).

## **PRESENTATIONS**

(presenter underlined; undergraduate students denoted with asterisk; graduate students denoted with two asterisks)

1. S. Krawczyk\*, B. F. Gherman, E. C. Brown. "Computational Analysis of Carbonic Anhydrase Biomimetic Reactivity via Novel Metal-Hydrosulfide Complexes." (poster) 24<sup>th</sup> California State University Biotechnology Symposium; Santa Clara, California; January 2012.
2. S. J. Bertolani\*, A. E. Zamora\*, B. F. Gherman. "Computational Study of Hydrogen Bonding Residues and Thiolate Coordination in the Active Site of Eubacterial Peptide Deformylase." (poster) 24<sup>th</sup> California State University Biotechnology Symposium; Santa Clara, California; January 2012.
3. S. Krawczyk\*, B. F. Gherman, E. C. Brown. "Computational Analysis of Carbonic Anhydrase Biomimetic Reactivity via Novel Metal-Hydrosulfide Complexes." (poster) 43<sup>rd</sup> Western Regional Meeting of the American Chemical Society; Pasadena, California; November 2011. \*\*undergraduate poster presentation award.
4. S. J. Bertolani\*, A. E. Zamora\*, B. F. Gherman. "Computational Study of Hydrogen Bonding Residues and Thiolate Coordination in the Active Site of Eubacterial Peptide Deformylase." (poster) 43<sup>rd</sup> Western Regional Meeting of the American Chemical Society; Pasadena, California; November

2011. \*\*undergraduate poster presentation award.

5. J. S. Fell, D. M. Steele\*, B. F. Gherman. "Electronic Effects on the Reaction Mechanism of the Metalloenzyme Peptide Deformylase." (poster) 43<sup>rd</sup> Western Regional Meeting of the American Chemical Society; Pasadena, California; November 2011.
6. S. Krawczyk\*, B. F. Gherman, E. C. Brown. "Computational Analysis of Metal-Hydrosulfide Complexes Supported by a Novel Carbonic Anhydrase Biomimetic Ligand System." (poster) 23<sup>rd</sup> Annual Undergraduate American Chemical Society Research Conference for Northern California; San Jose, California; May 2011. \*\*awarded 1<sup>st</sup> place poster presentation.
7. R. Fernandez\*, N. Korovina\*, B. F. Gherman, J. D. Spence. "Computational Study of the Cyclization Reactions of Quinoxaline-Based Eneidyne." (poster) 23<sup>rd</sup> Annual Undergraduate American Chemical Society Research Conference for Northern California; San Jose, California; May 2011.
8. V. A. Mendiola\*, B. F. Gherman, J. A. Miranda. "Metal-Salens as Catalysts for the Reduction of Alkyl Halides: Analysis of Factors Affecting Reaction Pathway and Thermodynamics." (poster) 23<sup>rd</sup> California State University Biotechnology Symposium; Anaheim, California; January 2011.
9. J. S. Fell\*\*, D. M. Steele\*, B. F. Gherman. "Electronic Effects on the Reaction Mechanism of the Metalloenzyme Peptide Deformylase." (poster) 23<sup>rd</sup> California State University Biotechnology Symposium; Anaheim, California; January 2011.
10. B. F. Gherman. "Computational Study of the Cyclization Reactions of Naphthyl-Substituted Eneidyne." San Jose State University; San Jose, California; November 2010.
11. N. Korovina\*, B. F. Gherman, J. D. Spence. "Computational Study of the Cyclization Reactions of Naphthyl-Substituted Eneidyne." 22<sup>nd</sup> Annual Undergraduate American Chemical Society Research Conference for Northern California; Sacramento, California; May 2010.
12. V. A. Mendiola\*, K. A. Pineda\*, B. F. Gherman, J. A. Miranda. "Prediction of Reduction Potentials from Electron Affinities for Metals-Salens and Application to the Reduction of Alkyl Halides." 22<sup>nd</sup> Annual Undergraduate American Chemical Society Research Conference for Northern California; Sacramento, California; May 2010.
13. D. Steele\*, B. F. Gherman. "DFT Computational Study of Biomimetic Model for the Metalloenzyme Peptide Deformylase." (poster) 22<sup>nd</sup> Annual Undergraduate American Chemical Society Research Conference for Northern California; Sacramento, California; May 2010.
14. N. Korovina\*, B. F. Gherman, J. D. Spence. "Computational Study of the Cyclization Reactions of Naphthyl-Substituted Eneidyne." (poster) 239<sup>th</sup> American Chemical Society National Meeting; San Francisco, California; March 2010.
15. V. A. Mendiola\*, K. A. Pineda\*, B. F. Gherman, J. A. Miranda. "Prediction of Reduction Potentials from Electron Affinities for Metals-Salens and Application to the Reduction of Alkyl Halides." (poster) 239<sup>th</sup> American Chemical Society National Meeting; San Francisco, California; March 2010.
16. N. Korovina\*, B. F. Gherman, J. D. Spence. "Computational Study of the Cyclization Reactions of

- Naphthyl-Substituted Eneidyne.” (poster) 22<sup>nd</sup> California State University Biotechnology Symposium; Santa Clara, California; January 2010.
17. V. A. Mendiola\*, K. A. Pineda\*, B. F. Gherman, J. A. Miranda. “Prediction of Reduction Potentials from Electron Affinities for Metals-Salens and Application to the Reduction of Alkyl Halides.” (poster) 22<sup>nd</sup> California State University Biotechnology Symposium; Santa Clara, California; January 2010.
  18. N. Korovina\*, B. F. Gherman, J. D. Spence. “Synthesis and photoreactivity of 1,2-bis(naphthalene-1-ylethynyl)benzene: A combined experimental and computational investigation.” (poster) 238<sup>th</sup> American Chemical Society National Meeting; Washington, DC; August 2009.
  19. A. E. Zamora\*, B. F. Gherman. “Computational Study of the Effects of the Hydrogen Bonding Protein Environment on the Enzymatic Mechanism of Eubacterial Peptide Deformylase.” (poster) 238<sup>th</sup> American Chemical Society National Meeting; Washington, DC; August 2009.
  20. B. F. Gherman. “Using Computational Chemistry and Biomimetic Models to Investigate Catalysis and Enzyme Active Sites” Symposium on Learning and Industry Targeting Computational Chemistry Opportunities (Sylicco.09); University of California, Davis; Davis, California; July 2009.
  21. N. Korovina\*, B. F. Gherman, J. D. Spence. “Synthesis and photoreactivity of 1,2-bis(naphthalene-1-ylethynyl)benzene: A combined experimental and computational investigation.” (poster) Symposium on Learning and Industry Targeting Computational Chemistry Opportunities (Sylicco.09); University of California, Davis; Davis, California; July 2009.
  22. A. E. Zamora\*, B. F. Gherman. “Computational Study of the Effects of the Hydrogen Bonding Protein Environment on the Enzymatic Mechanism of Eubacterial Peptide Deformylase.” (poster) Symposium on Learning and Industry Targeting Computational Chemistry Opportunities (Sylicco.09); University of California, Davis; Davis, California; July 2009.
  23. V. A. Mendiola\*, K. England\*, H. Kaur\*, S. B. Bateni\*, A. R. Mitchell\*, A. T. Galatti\*, M. H. Vu\*, B. F. Gherman, J. A. Miranda. “Prediction of Reduction Potentials from Electron Affinities for Metal-Salens: A Dual Experimental / Computational Approach.” (poster) Symposium on Learning and Industry Targeting Computational Chemistry Opportunities (Sylicco.09); University of California, Davis; Davis, California; July 2009.
  24. N. Korovina\*, B. F. Gherman, J. D. Spence. “Synthesis and photoreactivity of 1,2-bis(naphthalene-1-ylethynyl)benzene: A combined experimental and computational investigation.” (poster) 21<sup>st</sup> Annual Undergraduate American Chemical Society Research Conference for Northern California; Moraga, California; May 2009.
  25. A. E. Zamora\*, B. F. Gherman. “Computational Study of the Effects of the Hydrogen Bonding Protein Environment on the Enzymatic Mechanism of Eubacterial Peptide Deformylase.” (poster) 21<sup>st</sup> Annual Undergraduate American Chemical Society Research Conference for Northern California; Moraga, California; May 2009.
  26. V. A. Mendiola\*, K. England\*, H. Kaur\*, S. B. Bateni\*, A. R. Mitchell\*, A. T. Galatti\*, M. H. Vu\*,

- B. F. Gherman, J. A. Miranda. "Prediction of Reduction Potentials from Electron Affinities for Metal-Salens: A Dual Experimental / Computational Approach." (poster) 21<sup>st</sup> Annual Undergraduate American Chemical Society Research Conference for Northern California; Moraga, California; May 2009.
27. T. C. Hatcher III\*, A. E. Zamora\*, B. F. Gherman. "Computational Study of the Enzymatic Mechanism of Eubacterial Peptide Deformylase via Functionalization of a Biomimetic Ligand." (poster) 21<sup>st</sup> California State University Biotechnology Symposium; Los Angeles, California; January 2009.
28. T. C. Hatcher III\*, A. E. Zamora\*, B. F. Gherman. "Computational Study of the Enzymatic Mechanism of Eubacterial Peptide Deformylase via Functionalization of a Biomimetic Ligand." (poster) 42<sup>nd</sup> Western Regional Meeting of the American Chemical Society; Las Vegas, Nevada; September 2008.
29. K. England\*, H. Kaur\*, A. R. Mitchell\*, A. T. Galatti\*, M. H. Vu\*, B. F. Gherman, J. A. Miranda. "Prediction of Reduction Potentials from Electron Affinities for Metal-Salens: A Dual Experimental/Computational Approach." (poster) 42<sup>nd</sup> Western Regional Meeting of the American Chemical Society; Las Vegas, Nevada; September 2008.
30. M. F. Brown\*, T. C. Hatcher III\*, B. F. Gherman. "DFT Study of a Biomimetic Model for the Metalloenzyme Peptide Deformylase: Is the Identity of the Metal Center Significant?" 236<sup>th</sup> American Chemical Society National Meeting; Philadelphia, Pennsylvania; August 2008.
31. T. C. Hatcher III\*, B. F. Gherman. "Computational Study of the Enzymatic Mechanism of Eubacterial Peptide Deformylase via Functionalization of a Biomimetic Ligand." (poster) 20<sup>th</sup> Annual Undergraduate American Chemical Society Research Conference for Northern California; Santa Clara, California; May 2008.
32. K. England\*, H. Kaur\*, A. R. Mitchell\*, B. F. Gherman, J. A. Miranda. "Prediction of Reduction Potentials from Electron Affinities for Metal-Salens: A Dual Experimental/Computational Approach." (poster) 20<sup>th</sup> Annual Undergraduate American Chemical Society Research Conference for Northern California; Santa Clara, California; May 2008.
33. B. F. Gherman. "DFT Study of a Biomimetic Model for the Metalloenzyme Peptide Deformylase: Is the Identity of the Metal Center Significant?" Shasta College; Redding, CA; April 2008.
34. B. F. Gherman. "DFT Study of a Biomimetic Model for the Metalloenzyme Peptide Deformylase: Is the Identity of the Metal Center Significant?" 48<sup>th</sup> Sanibel Symposium; St. Simons Island, GA; February 2008.
35. M. F. Brown\*, B. F. Gherman. "DFT Computational Study of a Biomimetic Model for the Metalloenzyme Peptide Deformylase." (poster) 20<sup>th</sup> California State University Biotechnology Symposium; Oakland, California; January 2008.
36. K. England\*, H. Kaur\*, A. R. Mitchell\*, B. F. Gherman, J. A. Miranda. "Prediction of Reduction Potentials from Electron Affinities for Metal-Salens: A Dual Experimental/Computational

- Approach.” (poster) 20<sup>th</sup> California State University Biotechnology Symposium; Oakland, California; January 2008.
37. B. F. Gherman. “DFT Computational Study of a Biomimetic Model for the Metalloenzyme Peptide Deformylase.” California State University, Chico; Chico, CA; October 2007.
  38. M. F. Brown\*, B. F. Gherman. “DFT Computational Study of a Biomimetic Model for the Metalloenzyme Peptide Deformylase.” (poster) Symposium on Learning and Industry Targeting Computational Chemistry Opportunities (Sylicco.07); University of California, Davis; Davis, California; July 2007. \*\*awarded best *ab initio* molecular modeling poster.
  39. M. F. Brown\*, B. F. Gherman. “DFT Computational Study of a Biomimetic Model for the Metalloenzyme Peptide Deformylase.” (poster) Nineteenth Annual Undergraduate American Chemical Society Research Conference for Northern California; Rohnert Park, California; May 2007.
  40. B. F. Gherman, W. B. Tolman, and C. J. Cramer. “Evolution of Biomimetic Ligands for Modeling Dioxygen Activation at Monocopper Enzyme Sites.” (poster) Twelfth International Congress of Quantum Chemistry; Kyoto, Japan; May 2006.
  41. B. F. Gherman, W. B. Tolman, and C. J. Cramer. “Computational Modeling of Catalysis in Monocopper Enzymes: Dopamine  $\beta$ -Monooxygenase and Peptidylglycine  $\alpha$ -Hydroxylating Monooxygenase.” *Metalloprotein Interest Group*; University of Minnesota; Minneapolis, Minnesota; March 2006.
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